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## Diamond Quantum Nanoemitters 150113

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PONTIFICIA UNIVERSIDAD CATOLICA DE CHILE

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<b>14. ABSTRACT</b> <p>As final results of this project there are: (1) the investigation of the effect of phonons on the optical properties of solid state emitters. A microscopic model was developed to calculate the phononic spectral density function responsible for the optical line shape of colour centres in diamond and alike impurities in large-bandgap materials (PHYS REV B 94, 134305 (2016)); (2) the exploration of the coupling between strain and electronic charge in mechanical resonators using a single quantum emitter in diamond. The work was a collaboration with the Department of Physics at University of California, Santa Barbara. The work was published in PHYS. REV. APPL. 6, 0340055 (2016). (3) the investigation of several noise sources, magnetic and electric, on the relaxation time of electronic spins associate to colour centers in diamond. It was found that the relative sensitivity to magnetic and electric noise can be adjusted by external magnetic fields (PHYS REV B 93, 024305 (2016)); (4) the use of electronic spins as sensors of the local nuclear spin polarisation in diamond. Novel spectroscopical techniques were developed in order to obtain useful information about the nuclear bath (PHYS REV B 92, 241117R (2015)).</p>				
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# SCIENTIFIC REPORT

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## 1. Introduction

This 18-moth AFOSR project allowed us to explore several aspects of color centers in solids such as the engineering of the optical properties of single emitters in large band gap materials and the understanding of the effect of external perturbations such as electronic and magnetic noise on the relaxation process of electronic spins associated to impurities. Such understanding has allowed us to take advantage of the great control that is possible to achieve of the internal degrees of freedom and use them to implement novel sensors of small perturbations such as the magnetic field produced by nuclear spins and the strain caused by mechanical resonators that are made out of the same material that host these single emitters.

In what follows we list the main results and undergoing research.

## 2. Results

### 2.1 Microscopic modeling of the effect of phonons on the optical properties of solid-state emitters

Published in	PHYSICAL REVIEW B 94, 134305 (2016)
Authors	Ariel Norambuena [1,2], Sebastian A. Reyes [1,2], Jose Mejia-Lopez [1,2], Adam Gali, [3,4] and Jeronimo R. Maze[1,2]
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### Summary

Understanding the effect of vibrations in optically active nanosystems is crucial for successfully implementing applications in molecular-based electro-optical devices, quantum information communications, single photon sources, and fluorescent markers for biological measurements. Here, we present a first-principles microscopic description of the role of phonons on the isotopic shift presented in the optical emission spectrum associated to the negatively charged silicon-vacancy color center in diamond. We use the spin-boson model and estimate the electron-phonon interactions using a symmetrized molecular description of the electronic states and a force-constant model to describe molecular vibrations. Group theoretical arguments and dynamical symmetry breaking are presented in order to explain the optical properties of the zero-phonon line and the isotopic shift of the phonon sideband.

See Appendix 1 for more information.

## 2.2 Strain Coupling of a Mechanical Resonator to a Single Quantum Emitter in Diamond

Published in	PHYSICAL REVIEW APPLIED 6, 034005 (2016)
Authors	Kenneth W. Lee [1], Donghun Lee [1,2], Preeti Ovartchaiyapong [1], Joaquin Minguzzi [3,] Jero R. Maze [3] and Ania C. Bleszynski Jayich[1]
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### Summary

The recent maturation of hybrid quantum devices has led to significant enhancements in the functionality of a wide variety of quantum systems. In particular, harnessing mechanical resonators for manipulation and control has expanded the use of two-level systems in quantum-information science and quantum sensing. Here, we report on a monolithic hybrid quantum device in which strain fields associated with resonant vibrations of a diamond cantilever dynamically control the optical transitions of a single nitrogen-vacancy (NV) defect center in diamond. We quantitatively characterize the strain coupling to the orbital states of the NV center and, with mechanical driving, we observe NV-strain couplings exceeding 10 GHz. Furthermore, we use this strain-mediated coupling to match the frequency and polarization dependence of the zero- phonon lines of two spatially separated and initially distinguishable NV centers. The experiments demonstrated here mark an important step toward engineering a quantum device capable of realizing and probing the dynamics of

nonclassical states of mechanical resonators, spin systems, and photons.

### **2.3 Competition between electric field and magnetic field noise in the decoherence of a single spin in diamond**

Published in	PHYSICAL REVIEW B 93, 024305 (2016)
Authors	P. Jamonneau[1], M. Lesik[1], J. P. Tetienne[1], I. Alvizu[2], L. Mayer[1], A. Dreau[1], S. Kosen[1], J.-F. Roch[1], S. Pezzagna[3], J. Meijer[3], T. Teraji[4], Y. Kubo[5], P. Bertet[5], J. R. Maze[2] and V. Jacques[1,6]
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#### *Summary*

We analyze the impact of electric field and magnetic field fluctuations in the decoherence of the electronic spin associated with a single nitrogen-vacancy (NV) defect in diamond. To this end, we tune the amplitude of a magnetic field in order to engineer spin eigenstates protected either against magnetic noise or against electric noise. The competition between these noise sources is analyzed quantitatively by changing their relative strength through modifications of the host diamond material. This study provides significant insights into the decoherence of the NV electronic spin, which is valuable for quantum metrology and sensing applications.

### **2.4 Local probing of nuclear bath polarization with a single electronic spin**

Published in	PHYSICAL REVIEW B 92, 241117(R) (2015)
Authors	P. London [1] R. Fischer [1], I. Alvizu, [2], J. R. Maze [2] and D. Gershoni [1]
Affiliations	[1] Department of Physics, Technion, Israel Institute of Technology, Haifa 3200003, Israel [2] Departamento de Fisica, Pontificia Universidad Catolica de Chile, Santiago 7820436, Chile

## *Summary*

The effect of a polarized nuclear spin bath on the dynamical behavior of a single electronic spin is studied theoretically and experimentally. The polarization of a single nuclear spin modifies the spin-echo signal of its neighboring electronic spin. When the electronic spin is surrounded by a bath of polarized nuclei, the spin-echo signals manifest a characteristic frequency related only to the nuclear spins abundance and their collective polarization. This frequency is proposed as an indicator for the local nuclear bath polarization. We quantify the realistic experimental regimes at which the scheme is efficient. Our proposal has potential applications for quantum sensing schemes, and opens a route for a systematic study of polarized mesoscopical systems.

## **3. Undergoing research**

### **3.1 Use of diamond color centers for fluorescent markers of Amyloid beta fibrils**

We are currently exploring the use of color centers in diamond to mark amyloid beta compounds, which are believed to be a precursor of the Alzheimer disease. We have successfully functionalized the surface of 30-nm diameter nanodiamonds in order to penetrate biological barriers and to detect amyloid beta fibrils in the extracellular region.

## **4. Concluding remarks**

The AFOSR grant allowed us to explore several aspects of color centers in large bandgap materials. We developed a microscopic model to explore the effect of phonons on the optical properties of solid-state emitters. We calculated the phononic spectral density function responsible for the optical line shape of colour centres in diamond and alike impurities in large-bandgap materials. It was also possible to explore the coupling between strain and electronic charge in mechanical resonators using a single quantum emitter in diamond. We investigated several noise sources, magnetic and electric, on the relaxation time of electronic spins associate to color centers in diamond. It was found that the relative sensitivity to magnetic and electric noise can be adjusted by external magnetic fields. Finally, we use the electronic spin associate to the nitrogen-vacancy center in diamond as a sensor of the local nuclear spin polarisation in diamond. Novel spectroscopical techniques were developed in order to obtain useful information about the nuclear bath.

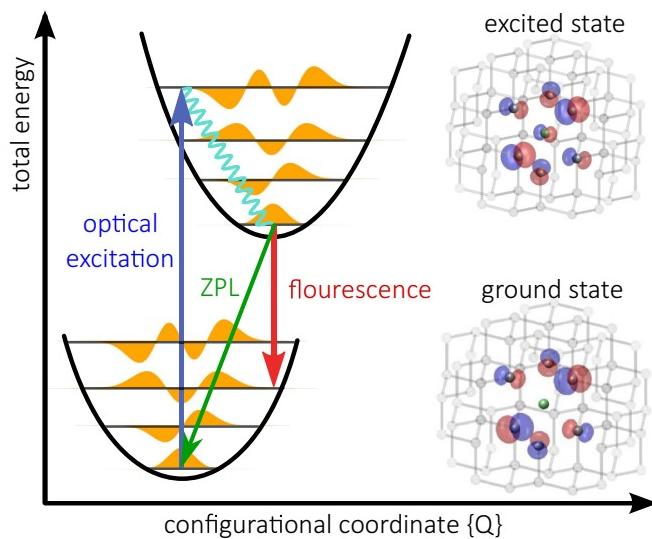
Jeronimo Maze  
Associate Professor  
Institute of Physics, Faculty of Physics  
Pontificia Universidad Catolica de Chile

## Appendix

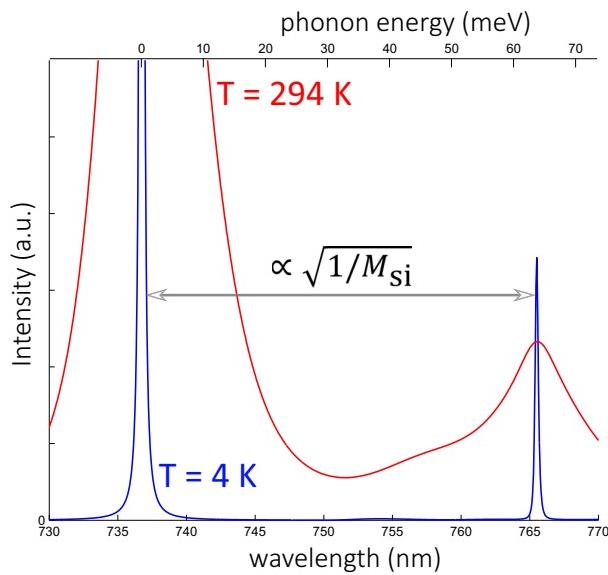
### A.1 Microscopic modeling of the effect of phonons on the optical properties of solid-state emitters

Here we describe the findings of the results published in PHYSICAL REVIEW B 94, 134305 (2016).

We have presented a microscopic model for estimating the emission spectrum of the SiV<sup>-</sup> using the Kubo formula and the spin-boson model. In addition we have considered effects to second order on the spectral density function via dynamical symmetry breaking. This spectral density function is estimated using a force-constant model for describing the vibrational modes and symmetrized electronic wave functions constructed using group theoretical arguments. This approach allows us to gain detailed insight on the microscopic origin and the role of symmetries on the emission spectra and the spectral density function, an approach which is crucially different from, but validates, phenomenological models presented in previous works. These results might be useful for understanding and engineering the optical properties of color centers in solids by extending the analysis to other deep and shallow centers coupled to phonons and subject to instabilities such as dynamic Jahn-Teller effects and external perturbations such as electric fields or strain.



**Figure A1.** Schematic representation of the potential energy diagram. The two parabolas represent the phononic potential of the ground  $e_{gx}$  and excited  $e_{ux}$  states of the SiV<sup>-</sup> including vibrational levels. Structure of the SiV<sup>-</sup> in diamond: six carbon atoms (dark gray) and the interstitial silicon atom (green) embedded in a diamond lattice (light gray). The molecular orbital representation of the electronic states  $e_{gx}$  and  $e_{ux}$  are represented by red (blue) for the positive (negative) sign of the electronic wave function.



**Figure A2.** Numerical emission spectra of the  $\text{SiV}^-$  in diamond. The blue and red curves represent the numerical emission spectrum obtained for  $T = 4 \text{ K}$  and  $T = 294 \text{ K}$ , respectively. The ZPL at 736 nm and the prominent sharp feature of the phonon sideband at 766 nm are reproduced. The peak at 766 nm is associated with the  $a_{1u}$  quasilocal phonon mode.